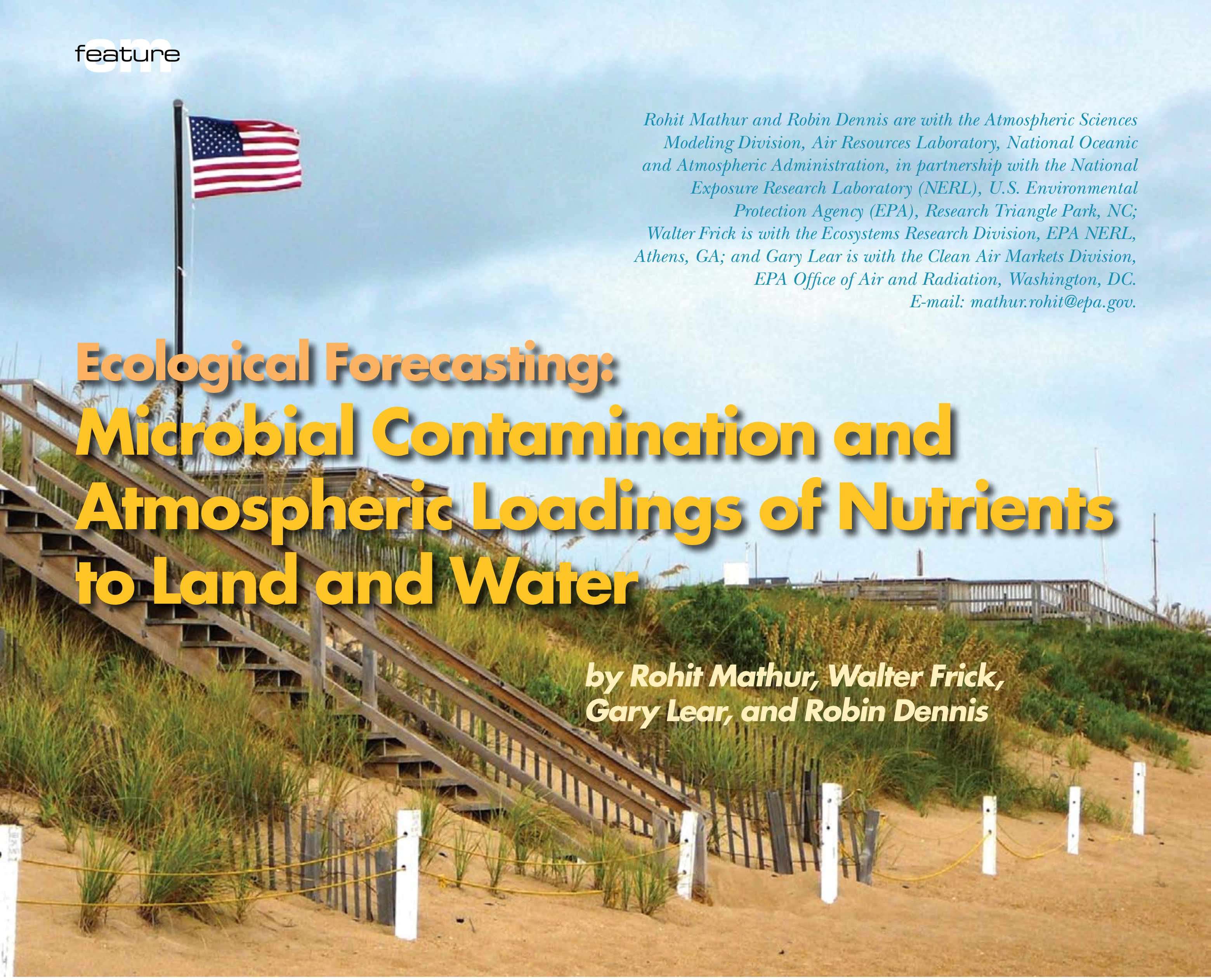

Rohit Mathur and Robin Dennis are with the Atmospheric Sciences Modeling Division, Air Resources Laboratory, National Oceanic and Atmospheric Administration, in partnership with the National Exposure Research Laboratory (NERL), U.S. Environmental Protection Agency (EPA), Research Triangle Park, NC; Walter Frick is with the Ecosystems Research Division, EPA NERL, Athens, GA; and Gary Lear is with the Clean Air Markets Division, EPA Office of Air and Radiation, Washington, DC. E-mail: mathur.rohit@epa.gov.

Ecological Forecasting: Microbial Contamination and Atmospheric Loadings of Nutrients to Land and Water

by Rohit Mathur, Walter Frick, Gary Lear, and Robin Dennis

Photo: The beaches of Corolla in the Outer Banks of North Carolina.

The development of ecological forecasts, namely, methodologies, to predict the chemical, biological, and physical changes in terrestrial and aquatic ecosystems is desirable so that effective strategies for reducing the adverse impacts of human activities and extreme natural events can be developed to sustain ecosystem productivity. The temporal and spatial scales of such ecological forecasts, in turn, depend on the ecosystem and the phenomenon being forecast. Since the development of comprehensive monitoring programs for ecological assessments and forecasting is expensive, scientists and environmental managers would need to increasingly rely on theoretical models for understanding nutrient effects and forecasting trends.[1]

Systems that include detailed descriptions of the pathways dictating the fate and transport of nutrients and contaminants from a combined atmosphere–land–water perspective are needed for integrated ecological assessments. Such systems must be able to accurately describe not only the cycling and residence time of contaminants in the individual media, but also the interactions from an integrated multimedia perspective. Significant efforts have been devoted over the past two decades toward the development of detailed models to address specific ecological problems. In recent years, several such efforts have been transitioned to provide short-term forecast of air and water quality. Linking the information from these evolving modeling systems could provide the building blocks for next-generation integrated ecological forecast models. Additionally, the development of continual archives of the model output from these systems could provide a vital long-term database, which, in conjunction with available monitored data, will help better characterize both short- and long-term responses of key ecological variables on spatial scales, ranging from local to continental.

FORECAST DEVELOPMENT

Air Quality Forecast Guidance Modeling System

Nitrogen is a key element, whose availability controls the productivity and functioning of many terrestrial

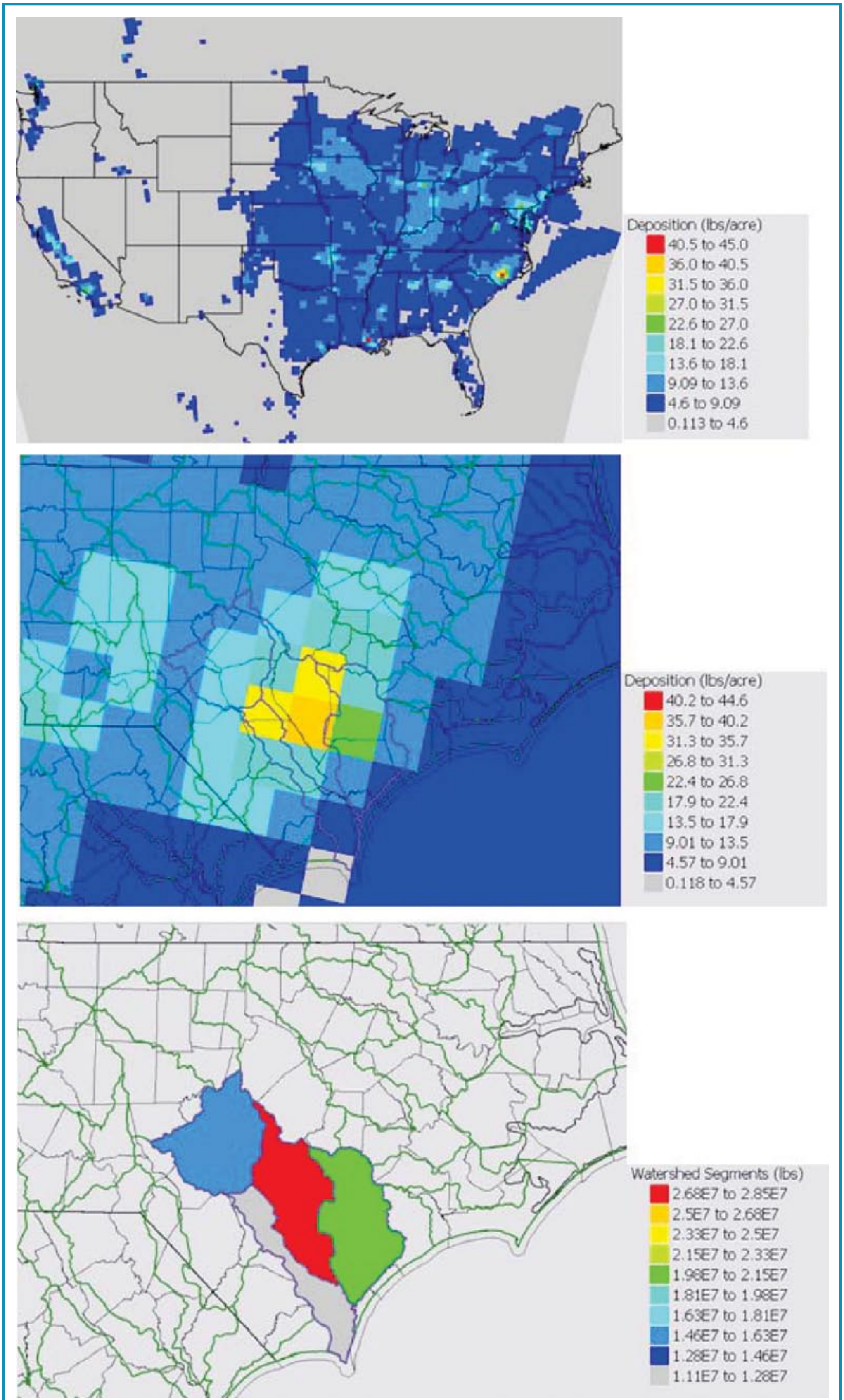

Figure 1. Mapping atmospheric nitrogen deposition estimates from the CMAQ model to watersheds using the Watershed Deposition Tool (WDT).[8]

Notes: The WDT calculates weighted average atmospheric deposition (wet, dry, or wet+dry) across a watershed or a set of watersheds.

and aquatic ecosystems.[1,2] Atmospheric deposition of nitrogen constitutes a significant source of externally supplied "new" nitrogen to sensitive ecosystems and is estimated to have grown 10-fold during the past century.[3] In ecosystems limited by nitrogen availability, it can enhance ecosystem productivity. By contributing to the exceedance of critical loads and imbalance in nutrient cycling, it may result in change in ecosystem diversity.[4] In freshwater and coastal regions, nitrogen deposition inputs can lead to variety of water quality and habitat degradation effects, such as harmful algal blooms, toxicity, fish kills, and ultimately loss of biodiversity.[4] As a source of nutrient input, atmospheric deposition is both a local and regional issue because sources of atmospheric nitrogen emissions may be situated within or outside the impacted ecosystem. Further, deposition could occur directly on to the sensitive ecosystem or indirectly (e.g., as deposition to a land surface with subsequent run-off) to a sensitive waterbody, the relative proportions of which in addition to its chemical composition can vary seasonally, depending on trends in emissions and prevalent weather conditions.

Comprehensive atmospheric models, by representing as much detail as possible about various dynamical, physical, and chemical processes regulating the fate of pollutants in the atmosphere, provide scientifically sound tools for developing air quality forecast guidance. In partnership with the U.S. Environmental Protection

Agency (EPA), the National Oceanic and Atmospheric Administration (NOAA) has deployed the initial stages of a national air quality forecast capability into NOAA's National Weather Service (NWS) operations to provide operational numerical air quality predictions (i.e., forecast guidance).[5] In this modeling system, numerical weather predictions by the NWS North American Mesoscale (NAM) model is linked operationally to the Community Multiscale Air Quality (CMAQ) model.[6] Detailed descriptions of atmospheric emissions of a variety of pollutants (including reactive nitrogen) based on the EPA National Emissions Inventory, along with three-dimensional descriptions of the changing dynamical state of the atmosphere derived from NAM, constitute the key inputs to the CMAQ model, which then simulates the spatial and temporal distributions of atmospheric pollutants as well as their distributions of wet and dry deposition amounts.

Currently, predicted ambient ozone concentrations are provided operationally on an hourly basis over a domain encompassing the Continental United States with a 12-km spatial resolution. Daily developmental particulate matter forecast simulations over the contiguous United States are currently underway to identify the challenges inherent in quantitative predictions of airborne fine particulate matter ($PM_{2.5}$). Findings from these evolving research and development activities will be transitioned into operational $PM_{2.5}$ forecast guidance systems over the next few years. Since nitrogen comprises a significant portion of the inorganic mass composition of ambient $PM_{2.5}$, and since the ultimate fate of oxidized (NO_y) and reduced (NH_x) nitrogen is the removal by wet scavenging and dry deposition onto terrestrial and aquatic ecosystems, output from these evolving and continuous forecast model applications can provide vital quantitative information on atmospheric nitrogen and acidic species deposition from hourly to annual scales over the contiguous United States. Figure 1a presents an illustration of annual total nitrogen deposition simulated by CMAQ.

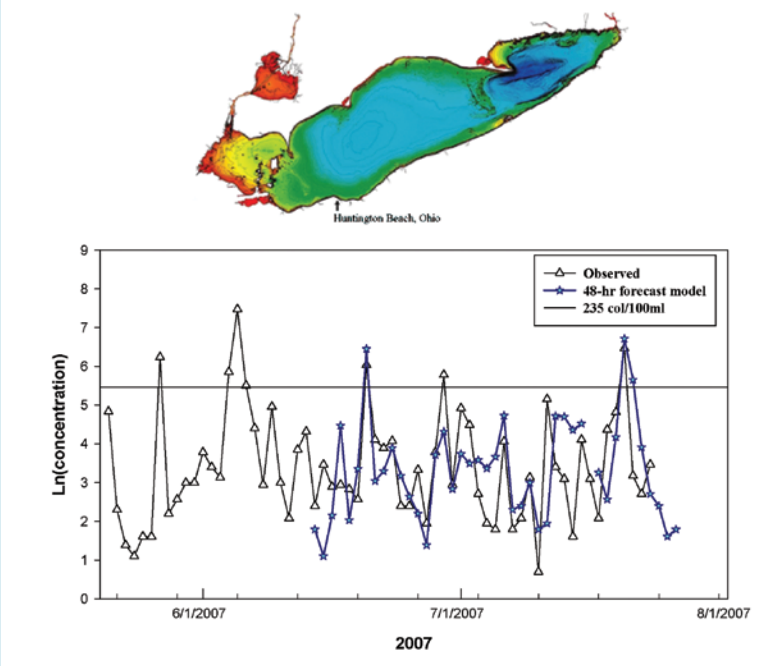

Figure 2. A comparison of *E. coli* 48-hr forecasts (stars) and observed concentrations (triangles) at Huntington Beach, OH, in summer 2007, relative to the 235-col/100-ml bathing water standard (horizontal line).

Notes: See www.ohionowcast.info/index.asp. The first forecast was made on June 10, 2007, for June 12, 2007, based on fitting to only 12 days of weather forecast data (starting May 30, 2007). For the sake of comparison with other models, the maximum number of variables was four, selected from 48-hr forecasts of temperature (°F), dewpoint temperature (°F), cloud cover (%), wind direction (deg), wind speed (mph), and precipitation potential (%) and the vector components of the wind, sometimes transformed. Except on days when bacteria data were delayed, subsequent model fits were based on an increasing number of days of data as bacteria measurements became available. This is called a dynamic modeling approach as compared to static models that are based on a fixed set of data (e.g., from a previous year). While some 48-hr tests were attempted in 2006, these are the first known published results. While the r^2 value is only 23.3%, it has been gradually improving and two of the three beach closures would have been correctly forecasted, with one false positive, overly protective forecast on July 21, 2007. Results such as these hopefully will help show that bacteria concentrations may be successfully forecasted in the same season that data are acquired, a quick-start approach to beach forecasting.

Water Quality Prediction and Forecasts

Beaches that meet water quality standards are valued for recreational and financial opportunities, as well as aesthetics. While pollution of surface water may not be obvious to most people, a day at the beach can make water quality degradation very apparent, if not visually, then through a subsequent visit to the pharmacy, or worse. To protect the public, beaches are subject to closure when bacterial counts exceed the water quality criteria. Beach closure decisions are often based on water samples that require a day to analyze. This is the basis of the persistence model: today's concentration is assumed to be the same as yesterday's. However, due to the variability in bacterial concentrations, this approach often yields many false positive and negative results.

Compared to predicting the fate and transport of simple conservative pollutants, such as metals, process-based bacteria modeling is extremely complex. Microbes, or bacteria, in the water column result from a myriad of point and nonpoint sources, large and small, proximate and distant. Many conditions and processes affect their distribution and fate directly, including nutrients, predation, solar radiation, sedimentation, resuspension, currents, density stratification, waves, temperature, and salinity. These, in turn, are affected indirectly by atmospheric conditions, such as atmospheric pressure, winds, temperature, humidity, sky conditions, and rainfall.

Persistence forecasts based on previous water samples often result in erroneous decisions.

Studies have shown that prognostic and empirical statistical models provide better results. Recognizing these challenges, EPA is developing a program called Virtual Beach, public-domain software for developing site-specific predictive models.[7] Virtual Beach includes multilinear regression concentration models that use real-time information on explanatory variables, such as turbidity, cloud cover, and rainfall, and has been shown to out-perform both simpler and complex models (see Figure 2). Virtual Beach could also be used to analyze stream nutrient concentrations, or even stock trends, as well as bacteria concentrations. Output from evolving weather and air quality forecast models could potentially provide valuable real-time information on the spatial and temporal variability of several key explanatory variables used in such water quality forecast models.

Persistence forecasts based on previous water samples often result in erroneous decisions.

MEASUREMENT DATA NEEDS AND OUTLOOK

The two primary monitoring networks for the characterization of atmospheric pollutant loadings to land and water surfaces are the National Atmospheric Deposition's National Trends Network (NADP/NTN) and the Clean Air Status and Trends Network (CASTNET). NADP/NTN was established in 1977 as a multi-agency cooperative network to monitor spatial and temporal trends in concentrations and deposition of major anions and cations in precipitation, and collects weekly precipitation samples for nutrients, including sulfate (SO_4^{2}), nitrate (NO_3^-) and ammonium (NH_4^+) ions. With more than 250 monitoring locations, the network has broad geographic coverage and includes sites in all major ecoregions of the United States. EPA established CASTNET in 1987 in anticipation of the Clean Air Act Amendments of 1990 for reporting on the effectiveness of air pollution control programs. It collects and analyzes weekly average concentrations of airborne sulfur dioxide, nitric acid, sulfate, nitrate, and ammonium, hourly concentrations of ozone, and hourly meteorological data at more than 80 stations across the United States.

Since direct measurements of dry deposition flux are difficult to obtain, fluxes are estimated using an inferential

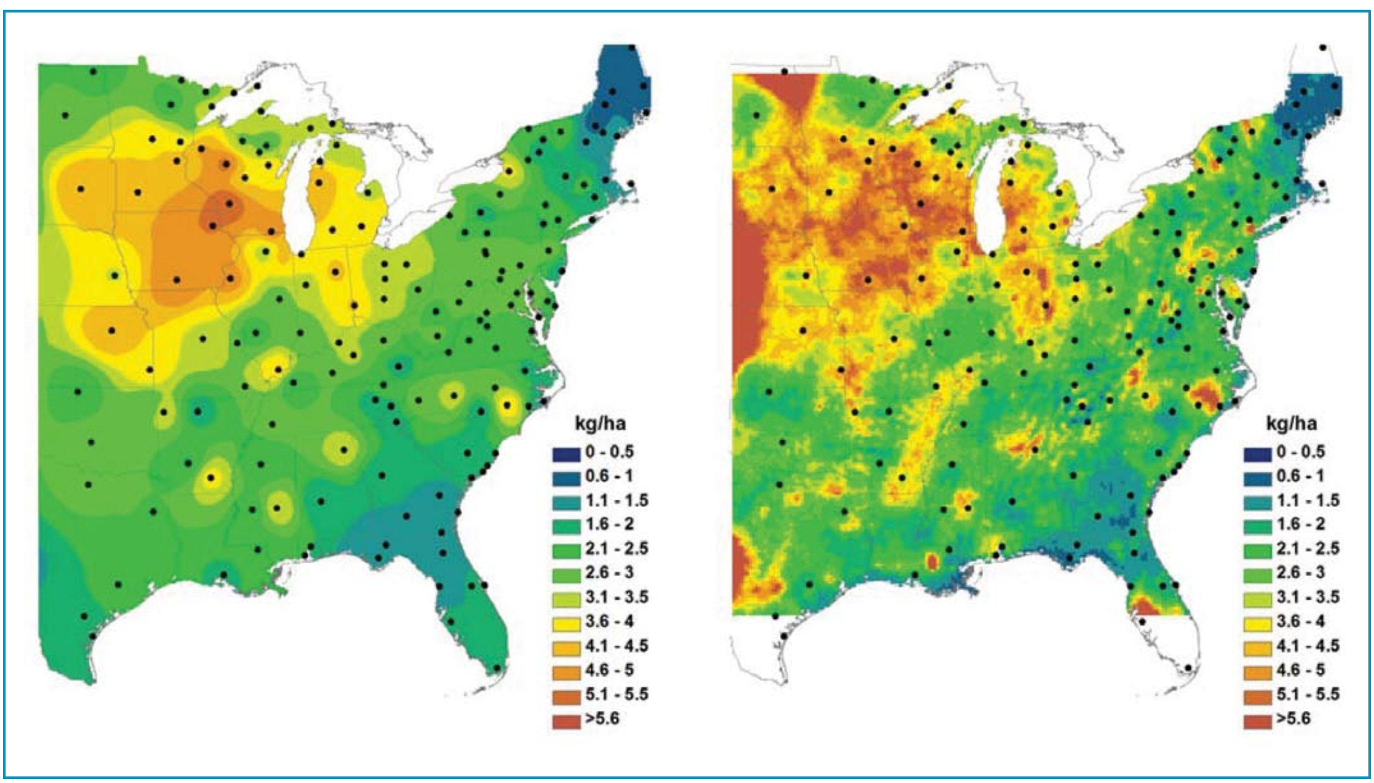

Figure 3. Illustration of the potential application of data fusion techniques to combine measured and modeled atmospheric deposition to develop enhanced maps of atmospheric nutrient loading.

Notes: Shown in these illustrations are annual observed NH_4^+ wet deposition fields derived from the NADP measurements (left) and fused observed and CMAQ derived fields (right) for 2001. The black dots represent location of the NADP monitors across the eastern United States. Interpolation of spatially sparse measurements cannot capture the inherent spatial variability in the deposition patterns. Fusing model and observed data provides opportunities to combine the relative strengths in models and observations to provide the best characterization of both ambient concentrations and deposition amounts.

model that combines ambient concentrations, meteorological data, and surface characteristics at the site. However, because dry deposition flux is inherently a surface phenomenon with actual deposition velocities determined by the microclimate and surface characteristics of the location, dry deposition estimates for individual sites are not necessarily valid across a heterogeneous landscape. Spatial variability and uncertainty are compounded in ecologically valuable landscapes because dry deposition processes in complex terrain and aquatic ecosystems are poorly understood.

While measurements from these networks have helped in characterizing long-term atmospheric deposition trends, their currently available speciation and spatial resolution limit the ability to develop accurate deposition surfaces based on measured data alone. Planned near-term enhancements to the CASTNET network, including measurements of ambient NH_3 and total NO_y, and the availability of these measurements in near real-time, will facilitate the use of these data in evolving ecological forecast modeling, as well as in the verification of the forecast models.

INTEGRATING MODELING DATA FOR ECOLOGICAL FORECASTING

There is a growing need for both short- and long-term forecasts to support proactive environmental management decisions. While significant progress has been made in recent years in forecasting specific environmental effects, opportunities exist to exploit the synergisms in these evolving activities to lay the foundation for future integrated ecological forecast systems. For example, similar to weather forecasts, operational air quality forecasts are now available to provide advance warning of poor air quality conditions. The resultant health advisories are routinely used to warn sensitive populations of the onset, severity, and duration of air pollution episodes, as well as to encourage the public and industry to reduce atmospheric emissions producing activities. Similarly, modeling tools of varying complexities are being developed to provide advance warning of poor water quality. In many cases, the output from one system constitutes key input parameters for another (e.g., information on atmospheric dynamical conditions from weather prediction models can provide real-time information on key explanatory variables used in existing water quality models). Similarly, since wet and dry deposition constitute key sink terms in the mass balance equations used in models designed to simulate ambient air quality, the output from existing and evolving air quality forecast models could provide estimates of atmospheric deposition of nitrogen and other constituents to aquatic and terrestrial ecosystems on a continuous basis.

The characterization of the changing chemical and biological state of the environment resulting from urban, industrial, and agricultural expansion in conjunction with evolving regulations directed toward improving the quality of both air and water poses a significant challenge. Recent evidence from modeling and measurement studies show a dramatic increase in nitrogen loading in several coastal environments of which atmospheric deposition is estimated to contribute a significant fraction.[3] To fully understand these multimedia dynamics and accurately forecast high nutrient loading events, it is imperative to quantify not only the wet and dry depositional fluxes on annual and shorter timescales, but also the composition (i.e., reduced vs. oxidized nitrogen) of the total nitrogen deposition. Recognizing the need to link air and water quality models to include atmospheric deposition in water quality estimates, a Watershed Deposition Tool has recently been developed that maps deposition estimates from air quality models to watersheds (see Figure 1).[8]

The continuous archival of the output from emerging forecast applications also provides opportunities to examine long-term trends and relationships between explanatory variables and both chronic and acute ecosystem impacts. For example, EMEP, a cooperative program for monitoring and evaluation of the long-range transmission of air pollutants in Europe, updates deposition maps for sulfur and nitrogen pollutants based on meteorology-driven theoretical models,[9] similar to those being deployed in air quality forecasting activities in the United States. These model-derived deposition surfaces can then potentially be further enhanced through "data-fusion" or re-analysis with available measured values providing detailed and updated maps of deposition amounts over monthly, seasonal, or annual time-scales (see Figure 3). The availability of these estimates, and the coupling with watershed or terrestrial ecosystem models, can then facilitate examination of a variety of questions related to the relative importance of indirect versus direct atmospheric deposition, its spatial variability within and among geographic regions, and the relative importance of composition versus total nutrient deposition in terms of biogeochemical response. A better understanding of these issues will lead to the development of robust integrated ecological forecasting tools for effective environmental management. **em**

REFERENCES

1. National Research Council. *Clean Coastal Waters: Understanding and Reducing the Effects of Nutrient Pollution*; National Academy Press: Washington, DC, 2000; available at www.nap.edu/catalog/9812.html.
2. Vitousek, P.M. et al. Human Alteration of the Global Nitrogen Cycle: Sources and Consequences; *Ecol. Appl.* **1997**, *7* (3), 737-750.
3. Paerl, H.W. Connecting Atmospheric Nitrogen Deposition to Coastal Eutrophication; *Envron. Sci. Technol.* **2002**, 323-326.
4. Phoenix, G.K. et al. Atmospheric Nitrogen Deposition in World Biodiversity Hotspots: The Need for a Greater Global Perspective in Assessing N Deposition Impacts; *Global Change Biol.* **2006**, *12*, 470-476; doi:10.1111/j.1365-2486.01104.x.
5. Wayland, R.; Davidson, P. Air Quality Forecasting and Health Advisory Warnings; *EM* **2006**, *September*, 30-33.
6. Otte et al. Linking the Eta Model with the Community Multiscale Air Quality (CMAQ) Modeling System to Build a National Air Quality Forecasting System; *Weather Forecast.* **2005**, *20* (3), 367-384.
7. Ge, Z.; Frick, W.E. Some Statistical Issues Related to Multiple Linear Regression Modeling of Beach Bacteria Concentrations; *Environ. Res.* **2007**, *103*, 358-364.
8. Dennis, R.; Schwede, D.B. The Watershed Deposition Tool: A Means to Link Atmospheric Deposition to Watersheds. Presented at the *5th Annual CMAS User's Conference, Chapel Hill, NC, October 16-18, 2006*.
9. Erisman, J.W.; Grennfelt, P.; Sutton, M. The European Perspective on Nitrogen Emissions and Deposition; *Environ. International* **2003**, *29*, 311-325.